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We made considerable progress toward developing a practical model of polarized light scattering from non-spherical particles. Mueller matrix elements for single particles and collections of randomly oriented spheres, helices, cubes, ellipsoids and cylinders calculated with the C-D approximation were compared with experimental measurements and with Mie calculations. Mie calculations were used to train an artificial neural network that predicts the size parameter of a scatterer based on its S34 matrix element. The success of this simple network is an important first step in our goal of predicting the optical properties, size parameter, and shape of the particles that make up the scattering medium from experimental measurements of light scattering.

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"An Analytical Model of Light Scattering from Marine Micro-organisms and Detritus"

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March 1, 1995 to February 29, 1996

An Analytical Model of Light Scattering from Marine Micro-organisms and Detritus

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Research Goals

To understand and quantify light scattering from ensembles of irregularly-shaped objects. To characterize the effect of ensembles of micro-organisms on the propagation of polarized light through sea water. To determine the feasibility of detecting particle orientation and to assess the importance of scattering to underwater imaging techniques and irradiance calculations.

Objectives

To develop a numerical or analytical model that predicts angle-dependent scattering of polarized light from ensembles of non-spherical marine organisms, detritus, and inorganic particulates. To verify and examine the validity and range of applications of the model by comparison with exact calculations and/or experimental results as appropriate. Specific tasks toward the objectives are: (1) to develop an artificial neural network to recognize features in the scattering matrix elements associated with the irregular shape of oceanic scatterers, and (2) to refine and enhance the coupled-dipole approximation method.

Approach

Our earlier efforts to understand and quantify light scattering in the ocean were concentrated on the calculation of the Mueller scattering matrix from optical properties of the scattering medium. In this approach, the polarization states of the incident and scattered light are described by four-element Stokes vectors and the effect of the scattering medium on the incident beam is described by the sixteen-element Mueller or scattering matrix. The Mueller matrix for a given medium contains all the information on optical properties, size parameter, and shape of the particles that make up the scattering medium. The Mueller matrix for light scattering by spherical particles is generally determined by Mie

calculations, but for irregularly-shaped particles, it must be determined from an approximation method such as the coupled-dipole approximation.[1,2]

Our efforts during the past year were focused on the inverse problem. That is, given the experimental values of the Mueller matrix elements, what are the optical properties, size parameter, and shape of the particles that scatter the light? This information is contained in the Mueller Matrix, but it is not a simple task to retrieve it. The pattern recognition and classification properties of an artificial neural network offer a unique approach to retrieving the information. An artificial neural network that could accomplish this task must be capable of distinguishing the features of light scattering due to particle size from those due to index of refraction or particle shape.

An artificial neural network is a number computing elements connected in parallel. Despite its provocative name, the artificial neural network does not necessarily mimic a network of biological neurons. It is a computing system made up of a number of simple, interconnected processing elements, sometimes called neurons or nodes, operating in parallel. The network may be 'hard-wired' (constructed of electronic components) or created by a computer simulation. The artificial neural network described in this report is a computer simulation using a Power Macintosh desk computer.

A given neuron (node) may have any number of inputs but it has only one output. Each input value to the neuron is given a weight. In the neuron or node, each value is multiplied by its corresponding weight and the results are summed over all of the input values. The result of the computation (a single number) is then passed to a transfer function. The transfer function may contain a bias that adds a degree of freedom in training the network. Several different types of transfer functions are used in neural network architecture. For example, the transfer function may restrict the output of the neuron to be either a zero or a one (hard-limit function), or a number ranging between zero and one (log-sigmoid function), or just a number proportional to the input number (linear function).

A number of identical processing elements functioning in parallel constitute a layer. The layer that receives inputs is called the *input* layer. It performs no function other than buffering the input signal. The network outputs are generated from the *output* layer. A layers whose outputs are passed to the next layer is called a *hidden* layer. The network is *fully connected* if every output from one layer is passed along to every node in the next layer. When weight adjustments are made in preceding layers of feed forward networks by "backing up" from outputs, the term *back propagation* is used. The back propagation allows for the training of a network to produce the correct output. The architecture of the artificial neural network we have selected for our light

scattering analysis is a fully connected, 2 hidden-layer, back propagation neural network.

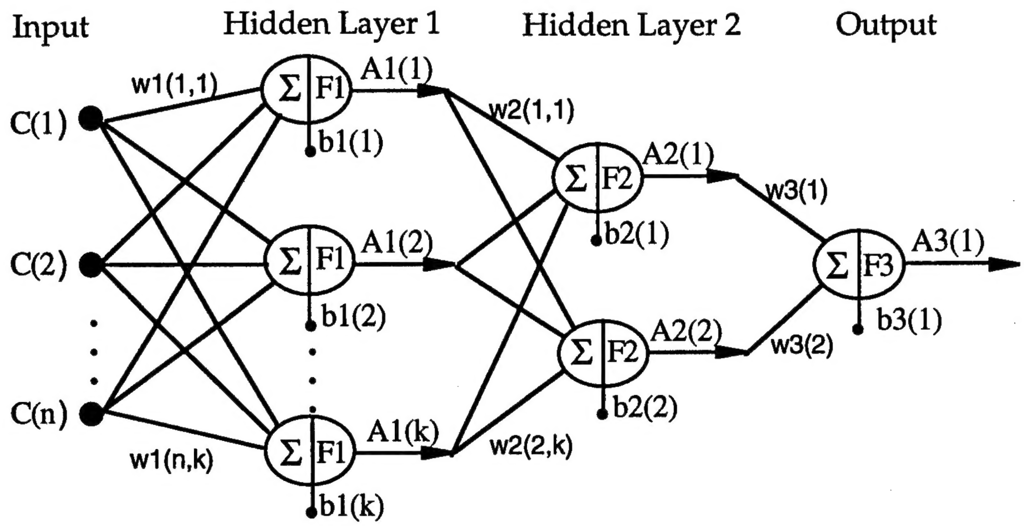

Figure 1. A multi-layer artificial neural network. The network shown is fully connected. There are n inputs values, k processing elements (nodes) in the first hidden layer, two nodes in the second hidden layer to distribute error, and one output node.

The initial approach to developing the desired neural net was to target one property of a scatterer, its size parameter. The size parameter is defined to be equal to $2\pi r/\lambda$, where r is the radius of the spherical particle and λ is the wavelength of the incident light in the medium. For non-spherical particles, r is taken to be the radius of a sphere of equivalent volume. The Mueller matrix element, S34, has been used to predict the sizes of bacteria,[3] so it seemed to be a good candidate for the input to the network. If the network is given the S34 matrix element as a function of scattering angle, can it determine the size parameter of the scattering particles? In order to construct a network that could be evaluated for different learning strategies and error determination methods, it was important to keep the number of input data points as small as possible so that the calculations could be carried out on a Macintosh computer. It has been shown that at least 3 or 4 processing elements for each input node (data point) is required for a network to have sufficient power to solve a problem of this type.[4,5] Fortunately, examination of the S34 matrix element calculated from Mie theory indicated that it could be duplicated extremely well with a Fourier series of as few as eight terms for size parameters up to about ten. Therefore, as much useful information about the functional form of S34 could be supplied to the network using the eight Fourier coefficients as with using forty or fifty data points. Instead of one or two hundred processing elements, a trainable network with as few as 24 processing elements was feasible. The final network design is similar

that shown in Figure 1 above. The network has eight input nodes (the Fourier coefficients) and one output node (the size parameter.) The first hidden layer has 32 nodes and the second hidden layer has 6 nodes. The output layer has a linear transfer function (F3 with a bias b3) and the two hidden layers both have log-sigmoid transfer functions (F1 and F2 with bias b1 and b2, respectively). Computations such as selection of initial weight matrices, summing weighted inputs (matrix inner product), calculations of the transfer functions, applying learning rules, and assessing the network's learning rate and performance were carried out using algorithms in the MATLAB library and its associated Neural Network Toolbox.[6] (MATLAB is a registered trademark of The Math Works, Inc.)

Tasks Completed

The development of computer codes for calculating the sixteen elements of the Mueller scattering matrix for a collection of randomly oriented particles was completed. Gaussian-Legendre integration over Euler angles was rigorously tested and proved to be a reliable method for calculating an orientational average of the Mueller matrix elements. Extensive calculations were made with the enhanced C-D model for collections of particles of various shapes including cylinders, cubes, prolate spheroids, hexagonal disks and helices. Spherical particles were also modeled so that comparisons could be made with Mie theory to assess limitations and ranges of application for the C-D calculations.

The design and initial training of an artificial neural network that predicts the size parameter of a light scatterer given its S34 matrix element was completed. As an alternative to experimental data, the network was trained and tested for both spherical and irregularly-shaped particles using Mie calculations and calculations made with the coupled-dipole model. The important features of a network are illustrated with this simple version. A more extensive network that predicts optical properties and shape factors, as well as size parameter, has also been designed. It does not differ in basic features from the simpler one, although it requires more input data and many more neurons to produce the desired results. We have shown that Mie and coupled-dipole calculations can provide a workable data set for training a neural network. However, it is important to test the network with experimental data. For this reason, future plans for this project include an experimental component at TSU to supplement the experimental work of Hunt and Quinby-Hunt at LBL.

During the summers of 1994 and 1995, the Principal Investigator and an undergraduate student worked with Arlon Hunt and Mary Quinby-Hunt at Lawrence Berkeley Laboratory. During this time, work was completed on a nebulizer system to produce aerosols similar to those found in the marine boundary layer. Angular-dependent Mueller matrix elements for the light

scattered by these aerosols were measured by Quinby-Hunt using the polarization-modulated nephelometer. In addition to the obvious value of experimental measurements in understanding the marine boundary layer directly, the measurements also serve as a data base to train and test the capability of the artificial neural network.

Scientific Results

Analytical Modelling of Light Scattering. The good agreement of the coupled-dipole calculations with both the Mie theory (Figure 2) and the experimental data (Figure 3) for light scattering from spheres at size parameters around five and possibly larger is promising. A size parameter of six translates into a particle size in the ocean of about one micrometer at visible light wavelengths. Many marine organisms and particulates of interest have sizes between one and two micrometers, putting them within, or close, to the current modeling limits of the coupled-dipole method. Differences between coupled-dipole and Mie calculations at large scattering angles indicates that the coupled-dipole model should be used with caution for scattering of visible light from irregularly-shaped particles much larger than one micron. The model could be employed, however, to predict trends or prominent features in the scattering. The comparisons between the experimental measurements of the scattering matrix elements of bacteria spores and the calculated values for similarly-shaped ellipsoids using the CD-approximation are shown in Figures 4 and 5. Although the comparisons are not good, some trends are evident. It is likely that the failure to obtain better agreement between the bacteria spores and the ellipsoids is due to the complex internal structure of the bacteria spore instead of its general shape.

The results of the comparison we have made between spheres (Mie Calculations) and ellipsoids (C-D calculations) of various aspect ratios provide an understanding of the degree to which non-spherical particles in the scattering medium effect the polarization state of the scattered light. (See Figure 6) In addition to this understanding, the results can also serve as a guide for determining when Mie calculations are adequate to describe scattering from a collection of particles and when we must use a model that includes scattering from non-spherical particles.

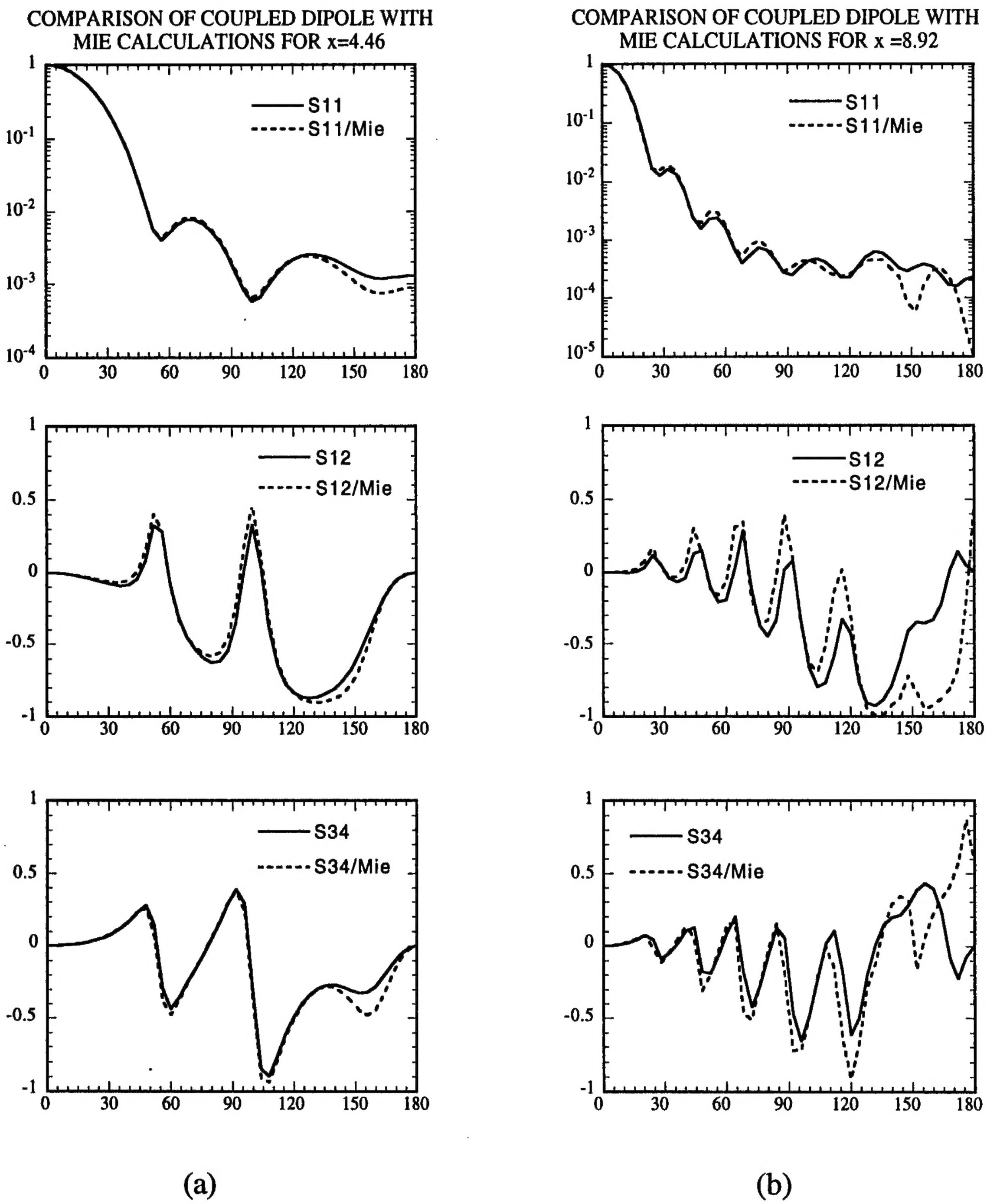

Figure 2. Comparison of the Mie calculations and the coupled-dipole approximation for spheres. The solid line represents coupled-dipole theory and dashed line represents Mie theory. Spheres with a size parameter of 4.46 are shown in column (a) and spheres with a size parameter of 8.92 are shown in column (b). In the coupled-dipole approximation, the sphere is modeled with 925 dipoles. In both calculations, the wavelength of incident light is 442 nm in air, the index of refraction of the medium (water) is 1.33, and the index of refraction of the sphere is 1.596.

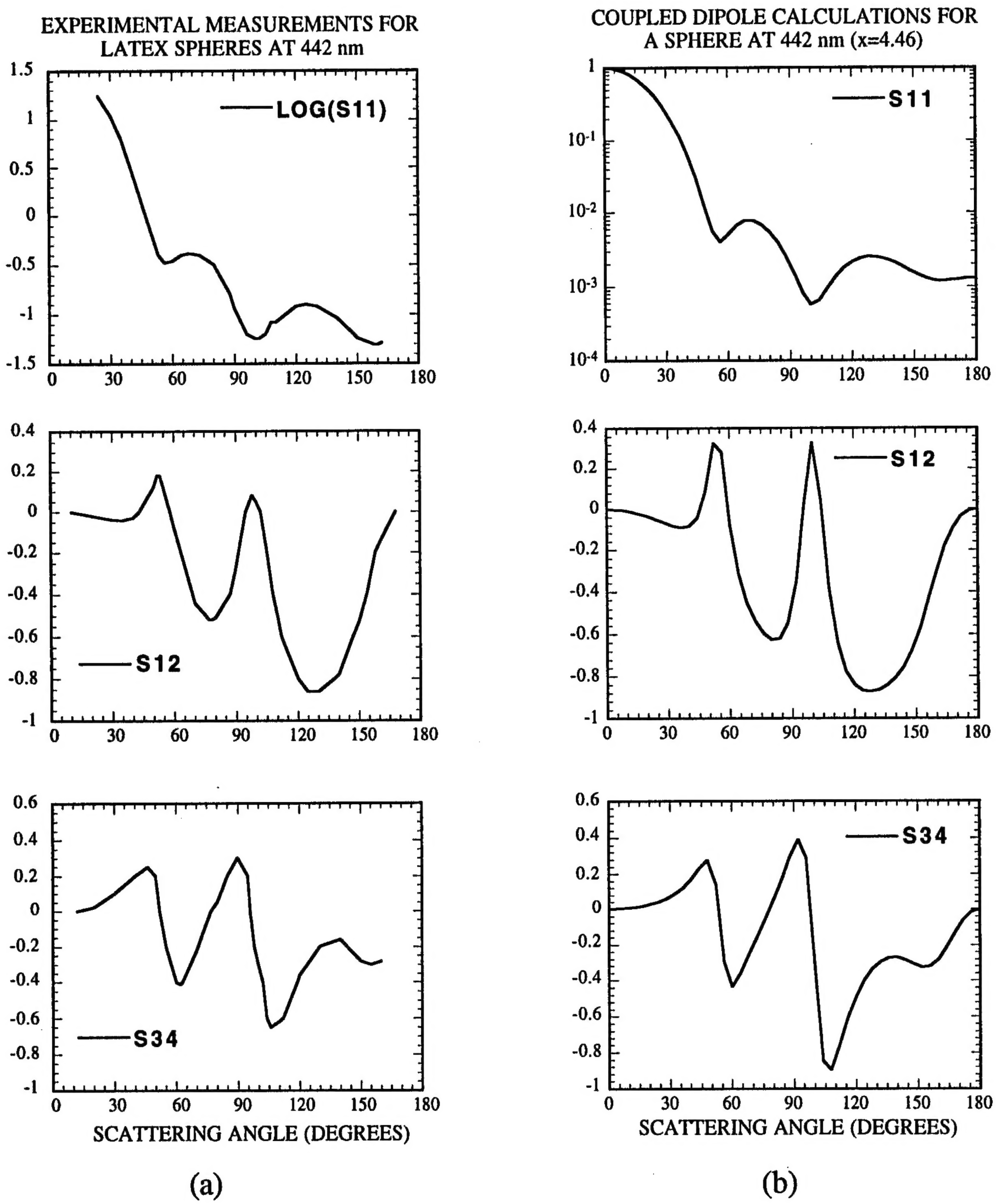

Figure 3. (a) Experimental measurements of the Mueller matrix elements for latex spheres. (b) Coupled-dipole calculations of the corresponding matrix elements for spheres of equivalent size parameter. In the coupled-dipole calculation, the sphere is modeled with 925 dipoles. In both figure, the wavelength of the incident light is 442 nm in air. The index of refraction of the medium (water) is 1.33 and the index of refraction of the sphere is 1.596.

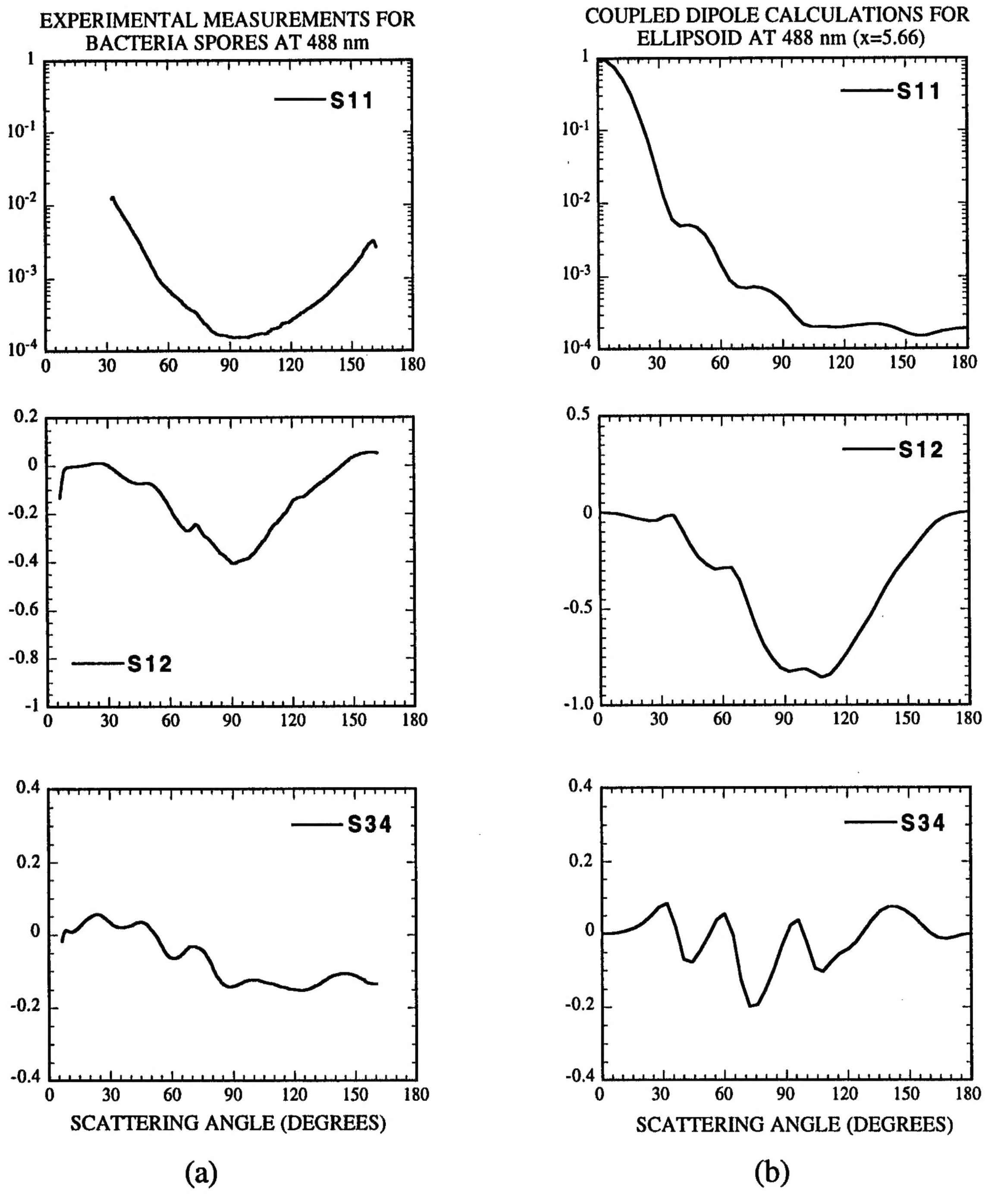

Figure 4. (a) Experimental measurements of the Mueller matrix elements for the *B. subtilus* spores. (b) Coupled-dipole calculations of the corresponding matrix elements for an ellipsoid. In the coupled-dipole calculations, the ellipsoid is modeled by 1032 dipoles and has a ratio of major to minor axis of 2.0. In both figures, the wavelength of incident light is 488 nm in air, the index of refraction of the medium (water) is 1.33 and the index of refraction of the ellipsoid is 1.48.

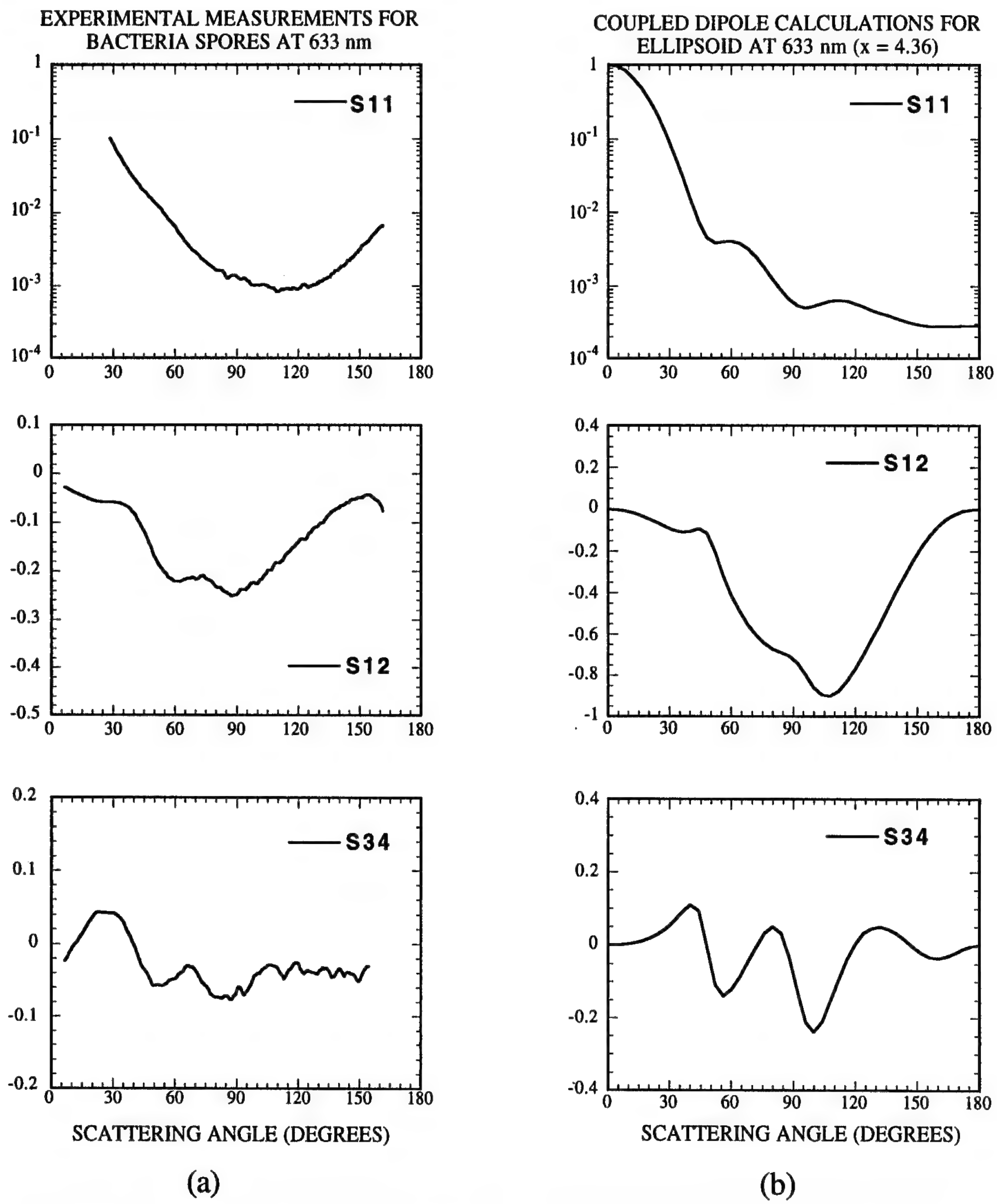

Figure 5. (a) Experimental measurements of the Mueller matrix elements for the *B. subtillus* spores. (b) Coupled-dipole calculations of the corresponding matrix elements for an ellipsoid. In the coupled-dipole calculations, the ellipsoid is modeled by 1032 dipoles and has a ratio of major to minor axis of 2.0. In both figures, the wavelength of incident light is 633 nm in air, the index of refraction of the medium (water) is 1.33 and the index of refraction of the ellipsoid is 1.48.

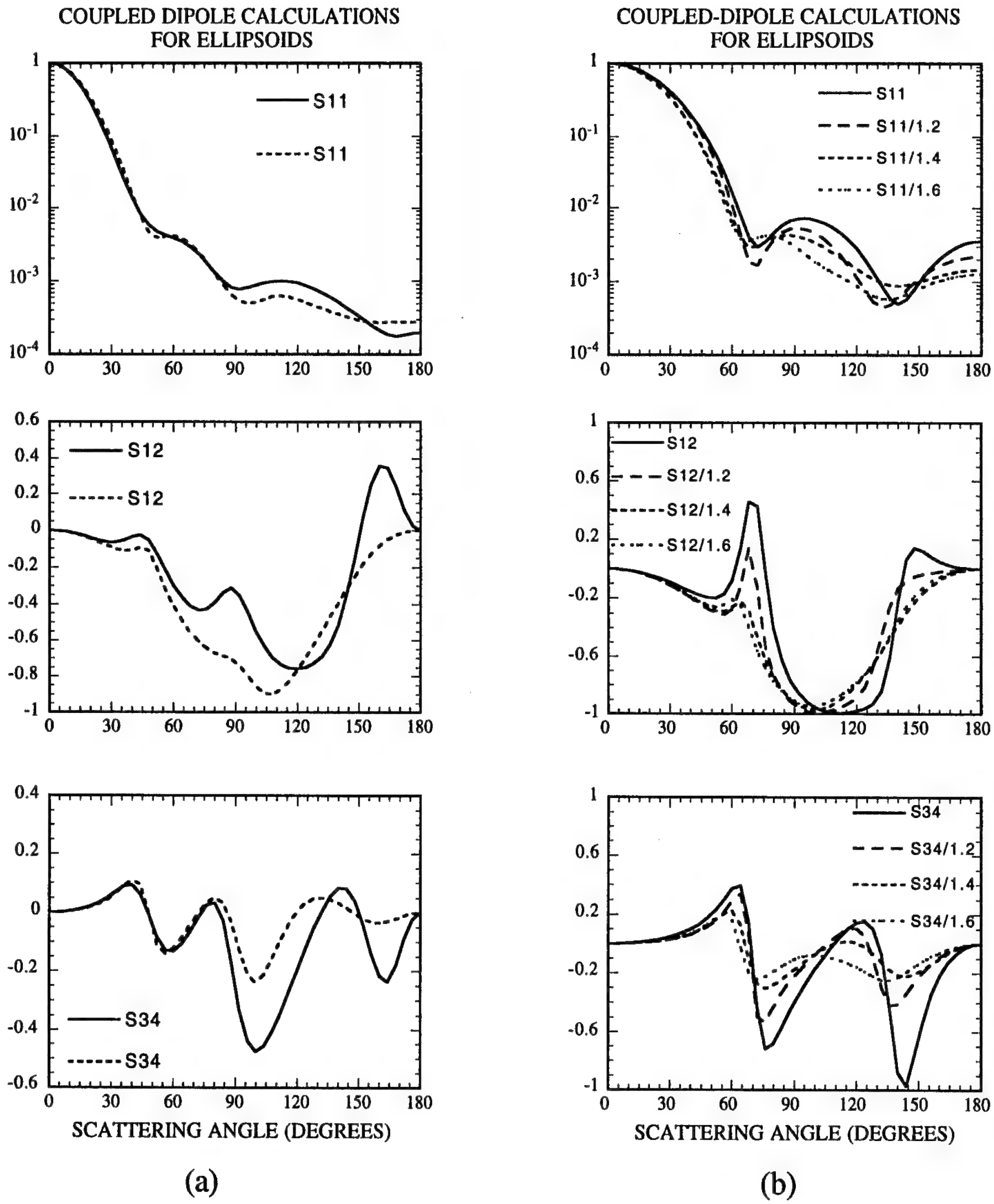

Figure 6. (a) Coupled-dipole calculations of the Mueller matrix elements for ellipsoids of two different values of the relative index of refraction. The solid line represents an ellipsoid with a relative index of refraction of 1.19 and the dashed line a relative index of refraction of 1.11. The size parameters are kept constant at 4.36 for both values of the relative index of refraction. (b) Mueller matrix elements for ellipsoids of varying ratios of major to minor axis. The solid line represents a sphere. Ratios of 1.2, 1.4 and 1.6 are labeled on each graph.

Neural Network Design. The original neural network was trained using a 'clean' data set determined from Mie theory. That is, the S34 matrix elements were calculated for a single sphere with a fixed index of refraction for size parameters ranging from one to ten. Size parameters less than one were not considered in the calculations since they are approaching the Rayleigh limit. Light scattering is not a function of particle size or shape in this limit. A 'clean' data set having a size parameter between two values in the original test set was presented to the network for analysis. The size parameter could be identified to within 1%, illustrating a neural network's ability to interpolate or generalize results.

Unlike calculated data, experimental data are often 'noisy.' In addition to the electronic noise in the instrument, the effects of scattering samples made up of a mixture of particles of different sizes, shapes and refractive indices contribute to the 'noise' in the data. A reasonable evaluation of a neural net cannot be made without taking into account 'noisy' input data. In order to simulate the features of experimental data, Mie calculations were made for a Gaussian distribution of spheres with varying indices of refraction and coupled-dipole calculations with orientational averaging were made for ellipsoids, cubes and cylinders for different size parameters and index of refraction. The resulting S34 matrix elements are shown as a function of scattering angle for particles of different size parameters, indices of refraction and shape in Figure 7. The figure clearly shows why S34 was chosen as a predictor of size parameter. Figures 7(a) and 7(b) illustrate the strong dependence of S34 on size parameter. The index of refraction is kept constant in both (a) and (b). Figure 7(a) also shows how rapidly S34 goes to zero in the Rayleigh limit. Figure 7(c) depicts the change in S34 as the index of refraction is changed while keeping the size parameter fixed. Finally, Figure 7(d) illustrates differences that might be expected in S34 for particles of different shapes.

The 'noisy' data (different shapes and relative refractive index) shown in Figure 7 were presented to the network to test the network's ability to distinguish size parameter from shape and index of refraction variations. It was necessary to train a second version of the neural net to be insensitive to the variations in S34 due to index of refraction. This was accomplished by including S34's calculated for different indices of refraction in the training set. The new network could predict the correct size parameter for different indices of refraction, generally to within 10%. The network could also correctly identify size parameter for cubes as well as spheres, but in identifying the size parameter for ellipsoids and cylinders the error was very large (greater than 30%). The number of training sets and/or the number of neurons can be increased to improve the network's performance, or other matrix elements (S11, S12 and S33) can be used as training as testing data.

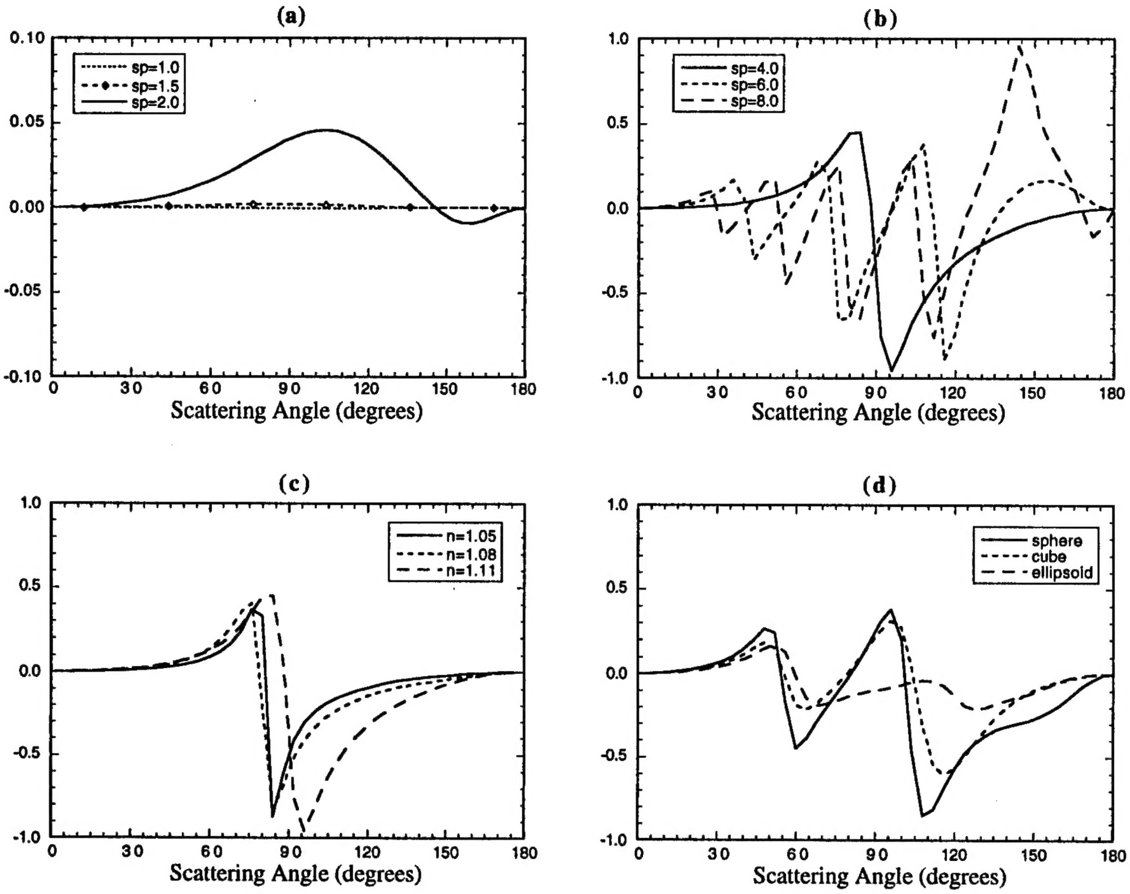

Figure 7. The Mueller matrix element, S34 as a function of scattering angle. (a) and (b) show S34 for spheres of various size parameters. (c) shows the variation of S34 for spheres with relative index of refractive for a constant size parameter, and (d) illustrates the effects of particle shape on S34. In all figures other than (c) the relative index of refraction of the scattering particles is kept constant at 1.11.

Accomplishments

We have made considerable progress toward developing a practical model of polarized light scattering from non-spherical particles. Mueller matrix elements for single particles and collections of randomly oriented spheres, helices, cubes, ellipsoids and cylinders calculated with the C-D approximation have been compared with experimental measurements and with Mie calculations. Since Mie calculations have been shown to accurately predict the scattering for marine organisms that are nearly spherical, comparisons of the results of Mie calculations with those obtained for irregularly-shaped particles using the C-D method helps to establish the limits of applicability of the Mie theory to non-spherical particles.

The artificial neural network is a unique and powerful tool that is being applied to large classes of problems. The tasks that the networks are performing in both

science and industry form an impressive list. In our inverse problem approach, a simple artificial neural network has been designed and tested that predicts the size parameter of a scatterer based on its S34 matrix element. The success of this simple network is an important first step in our goal of predicting the optical properties, size parameter, and shape of the particles that make up the scattering medium from experimental measurements of light scattering. Furthermore, the experience we have gained in designing, training and testing a neural network has given us insight into its potential applications. For example, existing light-scattering instruments could be modified to include a software version or a 'hard-wired' electronic version of a neural network that predicts size and optical properties of the scattering medium.

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